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19. ABSTRACT (Continue on reverse if necessary and identify by block number)

Work was accomplished in three areas:

A: Kinetic Energy of Products of Simple Ion-Molecule Reactions,

B: Generation and Reactivity of Carbon Cluster Ions,

C: Photodissouation Dynamics of Simple Ion-Neutral Clusters.

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Dr. Frank Wodarczyk	(202) 767-4960	NC

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Energy Disposal in Ion-Molecule Reactions

Michael T. Bowers
Department of Chemistry
University of California
Santa Barbara, CA., 93106

Grant No: AFOSR-86-~~0268~~ 0059
FINAL REPORT
15 November 1985 to 14 November 1988

I. ABSTRACT

During the tenure of this grant work was accomplished in the 3 areas listed in the OBJECTIVES section below. Summaries of this work have been given in the various Interim Reports and details of the published work are given in the attached set or reprints. In all, 13 papers have been published with the support of this grant and partial work completed on several other projects. The work has been presented at a large number of scientific meetings in both contributed and invited papers.

II. OBJECTIVES

A. Determination of Energy Disposal in Simple Bimolecular Reactions.

B. Determination of the Dynamics and Energy Disposal in the Photodissociation of Simple Cluster Ions.

C. Generation, Reactivity and Photochemistry of Carbon Cluster Ions.

III. PROGRESS

Summaries of the work done are given in the various interim reports on file. A more detailed summary of several aspects of the work can also be found in the proposal submitted in January, 1988 (and subsequently funded as Grant AFOSR–89–0102). Consequently a redundant summary of the work will not be given here. In the final few months of the grant progress was made on several new systems. These include photodissociation of CO_3^-, $CO_3^-.H_2O$ and Ar_3^+ and extension of some of our carbon cluster work. Papers are in the process of being written.

IV. PAPERS PUBLISHED OR IN PRESS

1985-1986

1. Photodissociation of Weakly Bound Ion-Molecule Clusters: $Kr{\cdot}SO_2^+$, H-S. Kim, M.F. Jarrold and M.T. Bowers, J. Phys. Chem. 90, 3584 (1986).
2. Photodissociation Dynamics of Negative Ion Clusters: $(SO_2)_2^-$, H-S. Kim and M.T. Bowers. J. Chem. Phys. 85, 2718 (1986).

3. Photodissociation Dynamics of Weakly Bound Ion-Neutral Clusters: $SO_2 \cdot O_2^+$, H-S. Kim, C-H. Kuo and M.T. Bowers, J. Chem. Phys. 86, 3283 (1987).

1986-1987

4. Photon Driven Charge Transfer Half-Collisions: The Photodissociation of $CO_2 \cdot O_2^+$ Cluster Ions With Resolution of the O_2 Product Vibrational States, H-S. Kim, C-H. Kuo and M.T. Bowers, J. Chem. Phys. 87, 2667 (1987).
5. The Mechanism and Product Energy Disposal in the Reaction of $C^+(^2P_u)$ with $O_2(X^3\Sigma^-)$, M. Rincon, J. Pearson and M.T. Bowers, Int. J. Mass Spectrom. Ion Proc. 80, 133 (1987).
6. A New Method for Studying Carbon Clusters in the Gas Phase; Observation of Size Specific Neutral Fragment Loss From Metastable Reactions of Mass Selected C_n^+, $n \leq 60$, P. Radi, T. Bunn, P. Kemper, M. Molchan and M.T. Bowers, J. Chem. Phys. 88, 2809 (1988).
7. Photodissociation Dynamics of Small Ionic Clusters: The $O_2^+ \cdot (CO_2)_2$ Trimer, H-S. Kim and M.T. Bowers,Int. J. Mass Spectrom. Ion Proc. 83, 71 (1988).
8. Product Energy Disposal in Simple Thermal Energy Bimolecular Ion-Molecule Reactions, M.T. Bowers and M. Rincon, Discussions Farad. Soc. 84, 303 (1987).
9. Intramolecular Energy Transfer Rates in Photoexcited Cluster Ions: The Photodissociation Dynamics of $CO_3^- \cdot H_2O$ and $CO_3^- \cdot CO_2$, J. Snodgrass, H-S. Kim and M.T. Bowers, J. Chem. Phys. 88, 3072 (1988).
10. "Ion Cyclotron Resonance Spectrometry; Experimental Methods", P. Kemper and M.T. Bowers, in Techniques of Chemistry, J.M. Farrar and W.H. Saunders (eds.), Wiley-Interscience, New York (1988).

1987-1988

11. Photodissociation Dynamics of $C_4H_6^+$ Ions from 1,3–Butadiene, T. Bunn and M.T. Bowers, J. Phys. Chem. 92, 1813 (1988).
12. The Mechanism and Product Energy Disposal in the Reaction of $Ar^+(^2P_{3/2})$ with $CS_2(X^1\Sigma_g^+)$, M. Rincon, J. Pearson and M.T. Bowers, J. Phys. Chem. 92, 4290 (1988).

13. Photodissociation Dynamics of Small Cluster Ions, M.T. Bowers in "Ion and Cluster Ion Spectroscopy and Structure," J.P. Maier (Ed.), Elsevier, Amsterdam (1980).

V. PERSONNEL ASSOCIATED WITH THE PROJECT

A. Senior Research Personnel

Dr. Paul Kemper
Dr. Petra von Koppen
Dr. Peter Radi
Dr. Thomas Bunn
Dr. Joseph Snodgrass

B. Junior Research Personnel

Ms. Hyun-Sook Kim
Ms. Marina Rincon
Ms. Coleen Roehl
Ms. Michele Molchan
Mr. John Pearson
Mr. Scott Lewis
Mr. Ming-Teh Hsu

VI. PAPERS PRESENTED AT MEETINGS

The various meetings at which both contributed and invited papers have been given on AFOSR sponsored research have been listed in previous interim reports. Here we list only a cumulative summary.

A. Contributed Papers at Scientific Meetings	21
B. Invited Papers at Scientific Meetings	14
C. Invited Seminars at Universities	9

AFOSR-TR- 89-0433

COMPLETED PROJECT SUMMARY

TITLE: Energy Disposal in Ion-Molecule Reactions

PRINCIPAL INVESTIGATOR: Professor Michael T. Bowers
Department of Chemistry
University of California
Santa Barbara, CA 93106

INCLUSIVE DATES: 15 November 1985 – 14 November 1988

CONTRACT/GRANT NUMBER: AFOSR-86-~~0268~~ 0359

COSTS AND FY SOURCE: $126,109 FY 86; $166,962 FY 87; $144,971 FY 88.

SENIOR RESEARCH PERSONNEL:
Dr. Paul Kemper
Dr. Petra van Koppen
Dr. Thomas Bunn
Dr. Chou-Hong Kuo
Dr. Joseph Snodgrass

JUNIOR RESEARCH PERSONNEL:
Ms. Hyun-Sook Kim
Ms. Marina Rincon
Ms. Michele Molchan
Ms. Coleen Roehl
Mr. John Pearson
Mr. Scott Lewis
Mr. Ming-Teh Hsu

PUBLICATIONS:

Photodissociation of Weakly Bound Ion-Molecule Clusters: $Kr{\cdot}SO_2^+$, H-S. Kim, M.F. Jarrold and M.T. Bowers, J. Phys. Chem. 90, 3584 (1986).

Photodissociation Dynamics of Negative Ion Clusters: $(SO_2)_2^-$, H-S. Kim and M.T. Bowers, J. Chem. Phys. 85, 2718 (1986).

Photodissociation Dynamics of Weakly Bound Ion-Neutral Clusters: $SO_2{\cdot}O_2^+$, H-S. Kim, C-H. Kuo and M.T. Bowers, J. Chem. Phys. 86, 3283 (1987).

Photon Driven Charge Transfer Half-Collisions: The Photodissociation of $CO_2 \cdot O_2^+$ Cluster Ions With Resolution of the O_2 Product Vibrational States, H-S. Kim, C-H. Kuo and M.T. Bowers, J. Chem. Phys. 87, 2667 (1987).

The Mechanism and Product Energy Disposal in the Reaction of $C^+(^2P_u)$ with $O_2(X^3\Sigma^-)$, M. Rincon, J. Pearson and M.T. Bowers, Int. J. Mass Spectrom. Ion Proc. 80, 133 (1987).

A New Method for Studying Carbon Clusters in the Gas Phase; Observation of Size Specific Neutral Fragment Loss From Metastable Reactions of Mass Selected C_n^+, $n \leq 60$, P. Radi, T. Bunn, P. Kemper, M. Molchan and M.T. Bowers, J. Chem. Phys. 88, 2809 (1988).

Photodissociation Dynamics of Small Ionic Clusters: The $O_2^+ \cdot (CO_2)_2$ Trimer, H-S. Kim and M.T. Bowers,Int. J. Mass Spectrom. Ion Proc. 83, 71 (1988).

"Ion Cyclotron Resonance Spectrometry; Experimental Methods", P. Kemper and M.T. Bowers, in Techniques of Chemistry, J.M. Farrar and W.H. Saunders (eds.), Wiley-Interscience, New York (1988).

Product Energy Disposal in Simple Thermal Energy Bimolecular Ion-Molecule Reactions, M.T. Bowers and M. Rincon, Discussions Farad. Soc. 84, 303 (1987).

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The Mechanism and Product Energy Disposal in the Reaction of $Ar^+(^2P_{3/2})$ with $CS_2(X^1\Sigma_g^+)$, M. Rincon, J. Pearson and M.T. Bowers, J. Phys. Chem. 92, 4290 (1988).

Photodissociation Dynamics of Small Cluster Ions, M.T. Bowers in "Ion and Cluster Ion Spectroscopy and Structure," J.P. Maier (Ed.), Elsevier, Amsterdam (1980).

ABSTRACT OF OBJECTIVES AND ACCOMPLISHMENTS:

Work was carried out in three areas under the support of this grant.

1. **Energy Disposal in Thermal Energy Bimolecular Ion-Molecule Reactions:**

Ion cyclotron resonance methods are used to accurately measure product kinetic energies in simple bimolecular ion-molecule reactions. These measurements allow determination of the electronic state distributions of the products and in favorable cases vibrational state distributions can be infered. Using state symmetry correlation diagrams and conservation of energy and angular monentum, much can be concluded about the details of the reaction mechanism. We have studied reactions of $C^+(^2P)$ with O_2 and OCS and $Ar^+(^2P_{3/2})$ with CS_2 and OCS.

2. **Photodissociation Dynamics of Simple Ion-Neutral Cluster Ions:**

We have developed a method for studying the photodissociation dynamics of mass selected ionic clusters. The mass selected beam is crossed by the polarized output of a laser and products mass and energy analysed. The technique allows measurement of product branching ratios, kinetic energy distributions, excited state lifetimes and symmetries and in favorable cases product internal state distributions, cluster bonding energies and qualitative cluster structures. In most cases substantial information is obtained on the detailed mechanism of the dissociation event. Systems studied include $Kr.SO_2^+$, $O_2^+.(CO_2)_2$, $O_2^+.CO_2$, $(SO_2)_2^-$, $CO^-_3.H_2O$ and $CO^-_3.CO_2$.

3. **Generation, Reactivity and Photochemistry of Carbon Cluster Ions:**

We have developed a laser desorption source for generating highly excited carbon cluster ions CN^+ and directly sampling the excited cluster distribution. Mass selected cluster beams undergo unimolecular decay in a field free region and then the product ions are mass and energy selected by a high resolution electrastatic analyser. Highly specific neutral loss is observed depending on cluster size; below n = 30 loss of C^3 dominates and above n = 30 only C^2 loss is observed. The work is being extended to careful analysis of product kinetic energy distributions, size specific reactivity studies and photodissociation.